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Initiative Director:

P. Michael Wright, Ph.D.
(208) 526-3315 or
wrigpm@inel.gov

For general information, or to be added to the mailing list, contact:
Steve Zollinger
(208) 526-9590
gaz@inel.gov

SubsurfaceTopics provides technical partners and interested researchers with information and updates about the INEEL's Subsurface Science Initiative and related research.



<http://subsurface.inel.gov/>



The INEEL's collaborative research efforts to study how fluids move in fractured rock have moved from large-scale field studies, such as at Box Canyon (above left) just outside the INEEL's boundaries, into the SSI's laboratories. Scientists are continuing their research with large instruments, such as the weighing lysimeter (above right).

INEEL Faces Fracture Flow Challenge

INEEL scientists believe research at a variety of scales is crucial in improving fundamental understanding of fluid movement in subsurface fractures.

The INEEL and Hanford sites share a characteristic in common with one-fifth of the nation's landfills tracked by the U.S. Environmental Protection Agency (EPA)—vulnerability—which results from their location in fractured rock areas. Though there is widespread concern about how quickly water and contamination can move through fractured

rock, the models currently used for predicting fracture flow inadequately reflect field and experimental realities. Researchers at the INEEL have been delving into the issue with a combination of research at a variety of scales and computational modeling approaches.

“Nearly half of the nation's drinking water comes from groundwater,” said Mike



INEEL hydrogeologist Thomas Wood (left) holds fractured basalt collected from the field. The basalt will be used in Wood's research—studying how fluids flow in fractured media—which is aimed at improving the accuracy of predictive models.

Wright, director of the INEEL Subsurface Science Initiative. “That fact, by itself, emphasizes why we need to better understand how contaminants move in fractured rock. Our research experience tells us that tackling the scaling issue is crucial in solving the problem of fracture flow.”

INEEL hydrogeologist Thomas Wood is leading one area of research. His team is examining how fracture intersections may integrate flow, a process that may cause flow paths to converge with depth.

“So far, the experimental results are definitely at odds with current models,” said Wood. He and his colleagues are proposing a fundamental shift in the conceptual model for fracture flow, a shift to combine better fundamental understanding of flow physics with the concept of mathematical complexity. (See *Fracture Flow Dynamics—The Building Blocks of Understanding Fractures* on page 3.)

Another INEEL research team is using stereolithography techniques to

study biofilms and learn how they affect fluid flow within simulated fracture systems. Their research has also required

“Our research experience tells us that tackling the scaling issue is crucial in solving the problem of fracture flow.”

— M. Wright,
director of the INEEL
Subsurface Science Initiative

them to develop techniques for measuring and modeling biofilm development. (See *Stereolithography Opens Window for Fracture Flow Study* on page 8.)

According to INEEL physicist Vance Deason, who conceived the idea of using optically transparent three-dimensional stereolithographs to model fracture systems, “Biofilms can potentially act as surfactants, reducing the surface tension of water and allowing it to flow more

easily through a fracture network. On the other hand, biofilms can grow in ways that physically block pores, causing reduced flow or switching of flow paths. A combination of experimentation and modeling is the only way to gain an understanding of how biofilms physically work.”

Besides iterating experiments and models, the SSI's research approach to improving understanding of fracture flow includes working across a wide variety of scales. (See *Crossing Scales to Understand Complexity* on page 5.) Mesoscale research not only offers a promising alternative to field-scale research, it may be the key to bridging the gap that currently separates laboratory understanding from the reality of the field.

“Decision-makers are being asked to take actions based on projections of contaminant locations thousands of years in the future over thousands of square kilometers,” said Randall LaViolette, an INEEL computational chemist. “Such requirements pose severe spatial and temporal scaling challenges to any model. The assumptions can only be tested directly with experiments of much shorter duration and smaller extent than the actual field situation. Therefore, mesoscale research is likely to play an important role in developing more realistic models.”

“We intend to find answers to the questions about fracture flow,” said Wright. “But to do that, we need to go beyond conventional modeling and laboratory approaches. We work across disciplines and across a range of spatial and temporal spatial scales. If we are serious about protecting groundwater resources, that is what we need to be doing.”

Contact: P. Michael Wright, Ph.D.
208-526-3315
wrigpm@inel.gov

Fracture Flow Dynamics—The Building Blocks of Understanding Fractures

Does water flow through fractures randomly or can patterns be predicted? An INEEL research team thinks the answer may be both. They intend to get a better idea by applying recent experimental results to a variety of new conceptual and computer models that accommodate the physics of flow and mathematical complexity. If they're right, their efforts will improve the accuracy of future predictive models.

"Water flowing through fractured rock above the water table appears to be integrated into discrete pulses caused by fracture intersections, not in the smooth wetting fronts assumed by current models," said INEEL hydrogeologist Thomas Wood. In his experiments of an idealized single fracture intersection, the water flow is similar to traffic flow at a street intersection. Just as traffic backs up when the light is red, water pools above a fracture intersection, held back by capillary forces. Gravity and, in some cases, inertia eventually overcome capillarity and the water pooled above the intersection is released to travel as a large pulse. The process then repeats. The discharge volume and frequency are dependent upon the flow rate and intersection geometry.

"Our hypothesis is that fractures tend to integrate flow in complex ways that current models don't account for," said fellow INEEL geoscientist Robert Podgorney.

Both Wood and Podgorney said their interest in fracture intersections was piqued after they got some unexpected results in an earlier experiment. That experiment, which replicated a simple fracture network with a stack of 12 limestone blocks, showed water paths converging at depth. (This experiment was

discussed in an article titled *Next Generation Vadose Zone Models* in the March 2002 issue of **Subsurface Topics**.)

In hopes of better understanding what they had seen, Wood, Podgorney and colleagues from several universities and from Sandia National Laboratories devised several simple experiments to explore the forces at play at intersections having different geometries. Their procedure uses smooth limestone bricks stacked and aligned in a cell. As water moves through the gaps between the bricks, which simulate fractures, a series of light sensors collects times-series data indicating the movement of water.

The initial four-brick experiment was enlightening. When water first arrived at an intersection, surface tension and capillary forces held it in place. Then, as the volume of water built up, capillary forces pulled it into the horizontal fracture. Eventually, the lens of water would contact a corner of the fracture, the volume would suddenly discharge and the process would begin again.

"What we observed seemed obvious, but it had never been described before,"

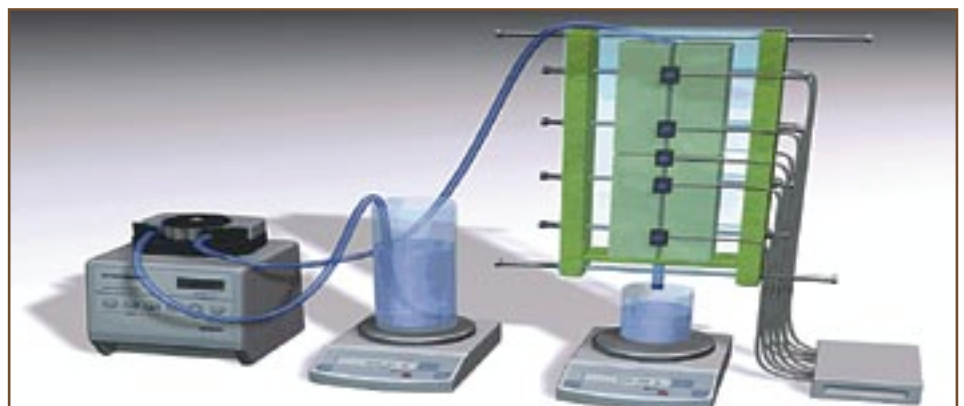
said Wood. "Fracture intersections serve as flow integrators."

The results of the four-brick experiment were analyzed to better understand both the physics and the mathematical dynamics of the system. So far, the team has determined that the volume discharged from the intersection remains relatively uniform at low flow rates. But at higher flows, it can be extremely variable if not chaotic. However, Wood believes the patterns from this and future experiments will eventually show emergent or complex behavior, rather than the signature of chaos. (See *Crossing Scales to Understand Complexity* on page 5).

The team also conducted variations on the experiment to study how the interaction of the various forces—such as capillarity, inertia and gravity—affected water accumulation and flow. Some of these included placing an obstruction at the intersection to disrupt the capillary forces. In others, the bricks were offset to create different horizontal flow regimes.

As other collaborators incorporate the new understanding of intersection physics into different computational models, Wood has moved onward to the next experiment.

The initial four-brick experimental setup for studying how water flows through fractured rock used four uniformly stacked limestone bricks to replicate a simple fracture network. A pump delivered a controlled flow of water to the top of the fracture and optical diodes were used to detect the presence of water pooling at various points in the fracture intersection.



“The four-brick apparatus is now being used to study how biofilms and periods of wetting and drying affect system behavior,” said Wood. “Fred White, a master technician on our team, and I are setting up a larger array of five

intersections. With that system, we can simultaneously monitor the interplay between multiple intersections.”

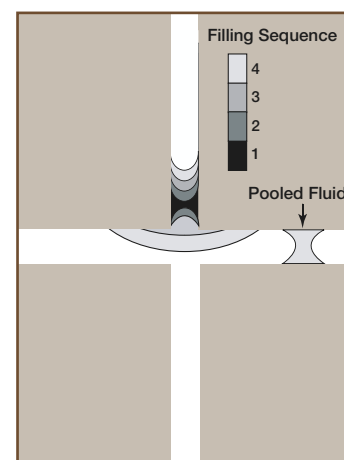
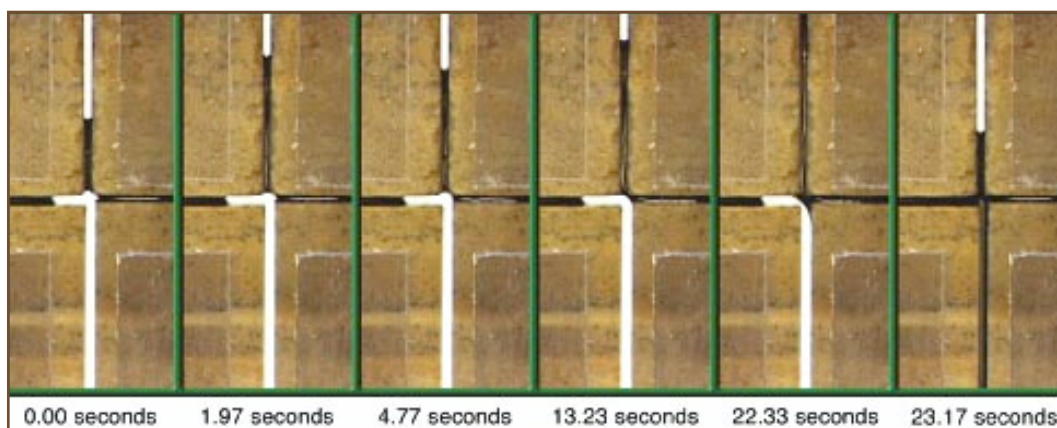
Wood hopes the larger experiment will further improve the team’s understanding of how fracture

intersections work together to integrate flow.

A report of the team’s initial observations about the physics governing fracture flow was recently published in the Dec. 15, 2002, issue of *Geophysical*

(Blocks continued on page 7)

The series of six photos (below) show how water arrives and moves through a fracture intersection in the four-brick experiment. The water builds up behind the intersection and simultaneously begins filling the horizontal fracture at its right. When the meniscus of water touches the opposing corner (next to last photo), it discharges. As the cycle repeats, small amounts of water can remain stored in the horizontal fracture. The diagram (right) illustrates the development of the meniscus.



Tipping Bucket Model Employed for Block Experiments

When it was time to build a useful model from data gathered in the four-brick fracture flow experiment, INEEL computational chemist Randall LaViolette turned to a model that conceptually seemed to be a good match. The model he chose is a well-understood mathematical construct known as a directed avalanche, or tipping bucket. LaViolette credits Robert Glass, a geohydrologist at Sandia National Laboratories, for the suggestion. Glass has spent years working on directed percolation models—one kind of which is the directed avalanche—to understand transport through fractured media.

To understand the basic concept of a tipping bucket model, imagine an array of buckets oriented into a diamond-shaped lattice. Any single bucket can tip and fill one of two buckets below. Likewise, any bucket can receive water from one of two buckets above. The buckets’ behavior is similar to the fracture intersections in the experiment—collecting and discharging water once they reach a certain threshold.

The four-brick experiment explored capillary forces, surface tension, inertia and gravity. Though these factors influencing the sudden release of water are complex, LaViolette believes the development of computational models must begin with simple assumptions. “A model should only allow for the minimum physical parameters necessary to explain a phenomena,” said LaViolette. “My goal is to isolate which factors are most critical in determining the discharge threshold.

“Since we are at the beginning stages, the initial model is coarse-grained,” said LaViolette. “Later, as our understanding improves, more parameters can be added to increase the model’s resolution.”

The model may need to account for other factors, such as microbes, minerals and contaminants, which can act as surfactants, sorbents or capillary inhibitors. As data come in from further experiments, LaViolette plans to incrementally revise the model as needed.

“Right now, the challenge is fitting the model to the first round of experimental data and the understanding of the physical forces at play,” said LaViolette.

Contact: Randall A. LaViolette, Ph.D.
208-526-1124
yaaq@inel.gov

Crossing Scales to Understand Complexity

Current predictive models for contaminant migration in the subsurface assume blobby, slow-moving plumes with even concentrations. So when scientists detect a contamination spike in a well, they expect that the entire contaminant plume is following close behind. In fractured rock systems, however, the expected plume often fails to materialize, leaving scientists scratching their heads. SSI researchers suspect that current models fail to account for mechanisms that may dominate the first arrival of contamination.

“In fractured rock systems, sporadic detections or detections far beyond the anticipated zone of influence defy current theory,” said INEEL geologist Thomas Wood. “The models we currently use to estimate the contaminant fate, including those specifically for fracture flow, underpredict these early arrivals.”

The INEEL’s fracture flow group is convinced that the isolated spikes are field confirmation of behavior observed in the laboratory. The group is delving into the issue by investigating how current models should evolve to represent the occurrence of the occasional spike in monitoring data and yet retain the “center of mass” type conceptualizations currently employed.

Just over a decade ago, predictive models for groundwater flow in fractured rock were full of uncertainty. Researchers from Lawrence Berkeley National Laboratory and the INEEL began to investigate how to impose more realistic limits on models and, in the years following, conducted several large-scale field studies in the fractured rock at and around the INEEL.

“The field studies produced huge amounts of data, which we use for calibrating and bounding today’s

groundwater models,” said Wood. “But field research is extremely challenging. It is expensive, there are few controls, not nearly enough instruments, and the data are very noisy.”

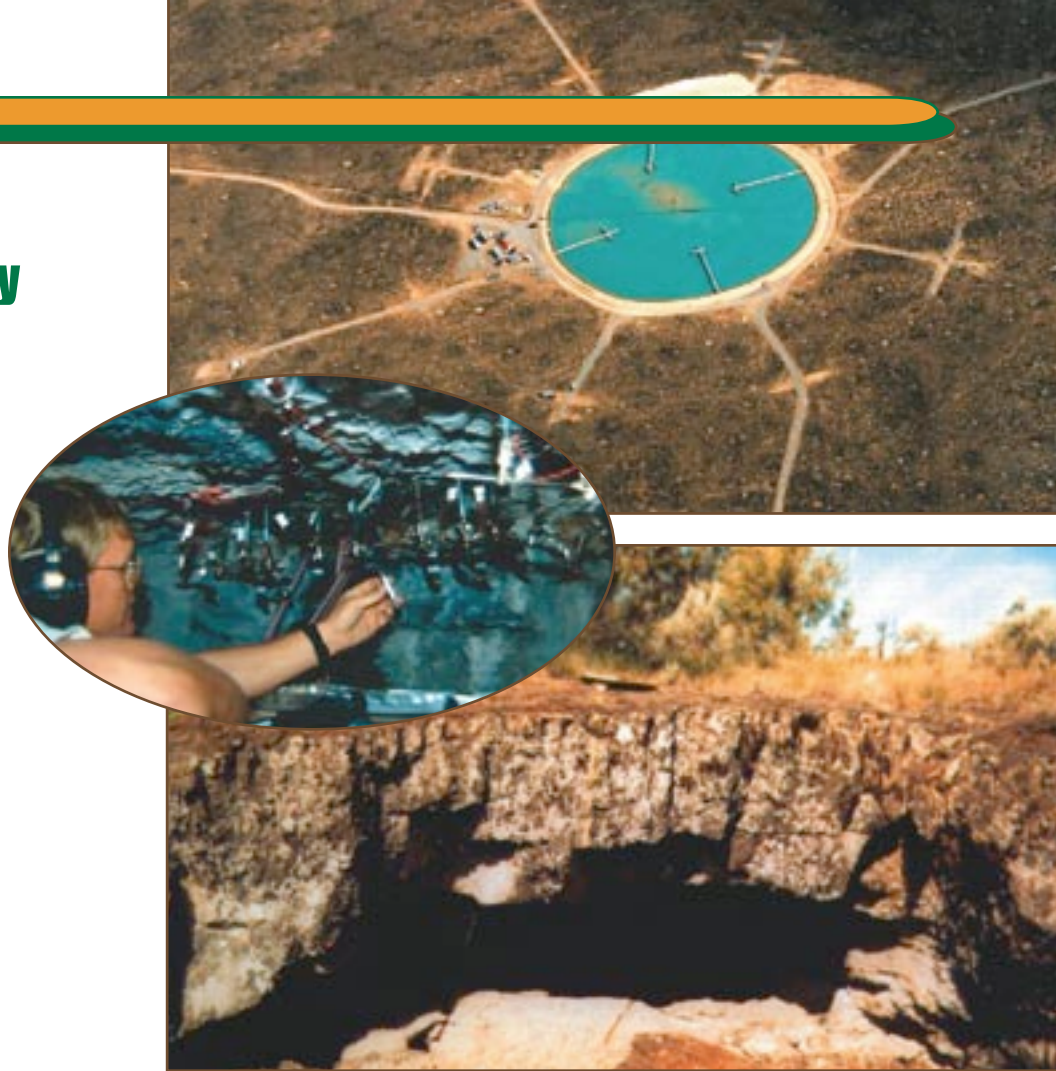
The first field studies, however, inspired INEEL to pursue fracture flow research. “We saw sudden events that no conceptual or computational model could account for,” said Wood. “We had no reasonable explanations. At one sampling event, an instrument would report dry conditions; at the next moment, it would be flooding.”

Wood and several colleagues conducted a smaller field experiment to examine a discrete fracture system. A meter-scale basalt overhang in southeastern Idaho’s Hell’s Half-Acre

lava field matched the experimental requirement.

Multiple experimental runs were conducted in which a known volume of water was placed in a pool on the surface and 20 sensors below the overhang recorded the time and location of the drips leaving the fracture. Researchers monitored temperature, humidity, flow rate, soil water pressure, and other variables, yet each trial yielded very different results despite apparently identical starting conditions.

“All my training and experience suggests that if the exact same thing is done repeatedly, the results should be fairly consistent,” said Wood. “But they weren’t.”

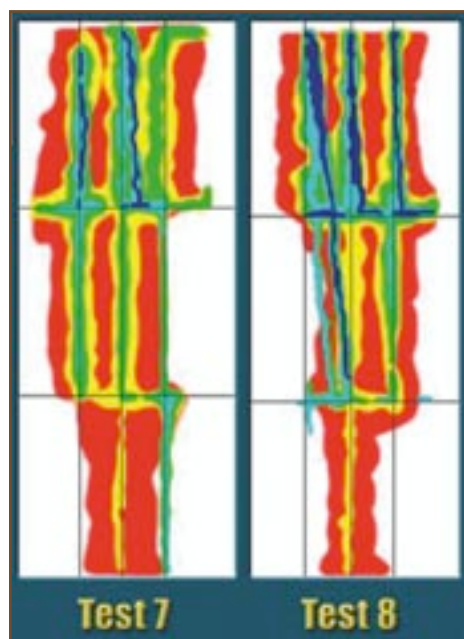


Changing experimental scales is the key to understanding the complex phenomena that scientists observed while conducting field experiments to investigate flow through fractured rock. Two of these field experiments were the Large-Scale Infiltration Test, which began in 1994 at the INEEL (top), and the Hell’s Half-Acre fracture flow study, which began in 1998 at a basalt outcrop adjacent to the INEEL (bottom).

Following the experiment, team member and Lawrence Berkeley hydrogeologist Boris Faybishenko showed that the system behaved chaotically. (See <http://www.esd.lbl.gov/ERT/projects/chaoticmods.html>). However, because of the team's continued work, Wood now favors another explanation. He believes the system showed emergent behavior characteristic of complexity. (See *Science Confronts Chaos and Complexity* on page 7.)

"The concepts of chaos and complexity are often at odds with traditional scientific thinking," said Wood. "Complex systems are capable of emergent behavior, where the larger-scale system differs from the sum of its smaller-scale component parts. The only way to study emergent behavior is to work across a variety of experimental scales."

INEEL researchers believe the convergence of flow observed in experiments replicating a simple fracture network is a behavior characteristic of complex systems. Images of wetted structure development in a stack of 12 limestone blocks (below) show the sequence of wetting at 7 min. 30 sec., 22 min. 49 sec., 50 min. 17 sec., 1 hr. 47 min., 3 hrs. 39 min. and 10 hrs. 9 min.



To pursue this possibility, the team decided to reduce the scale further and bring the experiments indoors. They set up a surrogate fracture network using a weighing lysimeter. (This experiment was discussed in *Next Generation Vadose Zone Models* in the March 2002 issue of **Subsurface Topics**.)

The experimental laboratory runs still do not repeat themselves in predictable ways, but the team saw definite patterns emerge at the mesoscale that echoed field observations: Though water flowing through a surrogate fracture matrix takes different paths, fracture intersections concentrate flow, causing it to converge with depth rather than diverge into smooth wetting fronts as current models predict. The results of this mesoscale experiment have been published in several journals.

Wood suspects the convergence of flow to be an emergent characteristic. "The problem with existing models is they assume that heterogeneities will average out if you consider large enough blocks of the subsurface," said Wood. "Instead, we are seeing an emergent behavior that appears to be amplified, rather than averaged, by heterogeneities. That's a characteristic of complexity."

Wood and his team think the stark contrast between their experimental results and the predictions of existing models is evidence of the need for revising the underlying conceptual models for fracture flow so new computational models can be developed.

"Right now, we're exploring a range of modeling approaches," said Wood. "But conceptually, all of them are capable of accommodating complex and emergent behavior."

Cellular automata models are one approach. These models treat heterogeneities as a system of cells, each governed by a set of rules. The rules, however, are not static, but change depending on the conditions of the cell and those in adjoining cells.

Geohydrologist and team member Robert Glass of Sandia National Laboratories has used a type of cellular automata model for simulating fluid flow in a single fracture. The results of his model show remarkable similarity to the behavior observed in laboratory experiments. Glass is expanding his work to include the effects of multiple fracture intersections acting in a network.

INEEL engineers and fellow team members Ray Berry and Rich Martineau are using a gridless particle-based modeling approach, which solves scaling issues using hydrodynamic numerical methods. In addition to being able to handle numerous fluid-solid and fluid-fluid interactions, other complexities can be simulated, such as multiple fluid phases and chemical, particulate and microbial transport.

Other approaches being considered also include directed avalanche models. (See *Tipping Bucket Model Employed for Block Experiments* on page 4.)

Wood suspects that developing experiments and models that factor in scaling and complexity will eventually produce models that more closely match field observations.

"Introducing the concept of complexity as a way to improve predictive capabilities seems like an oxymoron," said Wood. "But someday, I want to go back to our field data with a model capable of predicting what we observed. That would be very satisfying."

Contact: Thomas R. Wood
208-526-1293
tw@inel.gov

Note: This research is funded by DOE's Environmental Systems Research and Analysis program (ESRA). (The collaborators are the same as those for *Fracture Flow Dynamics—The Building Blocks of Understanding Fractures* on page 7.)

Research Letters. Wood and his colleagues are preparing a more detailed analysis for upcoming publication.

Contact: Thomas R. Wood
208-526-1293
tqw@inel.gov

Note: This research is funded by DOE's Environmental Systems Research and Analysis program (ESRA) and conducted by Thomas R. Wood, Daphne L. Stoner, Ph.D., Randall R. LaViolette, Ph.D., Robert C. Starr, Ph.D., Molly Leecaster, Ph.D., Timothy McJunkin, Robert K. Podgorney and

Karl Noah (all from the INEEL); Michael Nicholl, Ph.D. and Jerry Fairley, Ph.D. (University of Idaho); Robert J. Glass, Ph.D. (Sandia National Laboratory); David Peak, Ph.D. (Utah State University); and Douglas LaBrecque, Ph.D. (Multi-Phase Flow, LLC).

Science Confronts Chaos and Complexity

Chaos

In 1984, in the fairly new field of chaos theory, a classic study was performed at the University of California at Santa Cruz. The study demonstrated a pattern of chaotic behavior in a dripping water faucet. As INEEL physicist Paul Meakin observed, "If a dripping faucet can behave chaotically, it isn't too difficult to imagine fracture flow as potentially chaotic."

Meakin is working with Wood and others to explore complexity, chaos and fractal geometries in fracture flow. He recently gave an internal seminar on chaotic behavior and experimental reproducibility.

"When researchers can't reproduce a result, they often blame the technicians," said Meakin. "But there are a number of factors other than bad technique that can cause poor reproducibility, including chaotic behaviors."

Chaotic dynamics can wreak havoc with experimental reproducibility in even the simplest of systems and researchers often fail to consider their potential sources, especially in processes that are dominated by large rare events or with extreme sensitivity to conditions or perturbations. Among the chaotic dynamics that should be considered are noise amplification, proximity of experimental conditions to transitional states (such as a phase change), and system (or chaotic) intermittency.

Meakin explains chaotic intermittency by describing a familiar event—car trouble that disappears at the mechanic's shop and reappears when you drive the car away. If the time-varying behavior of the car is plotted, it will show long periods of repetitive, seemingly normal behavior and episodic aperiodic behavior that defies prediction or reproducibility. That time-varying behavior is known as a temporal fractal – the mathematical signature of chaos

As unpredictable as chaotic systems may be, it is possible to describe spatial and temporal fractals mathematically. The calculations required to identify patterns amidst chaos are highly repetitive and require intense computer processing. The biggest challenge is the number of measurements required, sometimes a quarter- to a half-million noise-free datapoints.

"It is not easy to prove a system is chaotic," said Wood. "You have to have patience and enjoy collecting data, tons of it."

Complexity

Though still not well defined, complex systems could be described as being composed of numerous, varied, simultaneously interacting parts. These parts consist of many independent constituents having structures that span several scales and interact in nonlinear ways.

Complexity, like chaos, is a shift away from reductive reasoning, where scientists believe an outcome can be predicted if all the factors are known. In

complex systems, patterns of behavior emerge that are often unpredictable and have unexpected outcomes that cannot be understood by an examination of the parts.

Emergent behavior is the defining characteristic of complex systems and is a phenomenon special to the scale considered. An emergent characteristic is one that can be observed at a higher scale, yet cannot be understood when its constituent components are individually studied at a smaller scale. For example, some fish form schools, yet this behavior would not be predicted by looking at individual fish.

The combination of structure and emergence in complex systems often leads to self-organization. This occurs when an emerging behavior has the effect of changing structures, often increasing the order of the system in defiance of the second law of thermodynamics.

Both complexity and chaos are dominated by nonlinearity, but they are very different. Chaos can occur in simple systems with very few constituents; complexity, by definition, cannot. However, complex systems can include components that behave chaotically.

Chaos can be discerned by gathering substantial experimental data and subjecting it to rigorous computational analysis. Complexity can be discerned by examining behavior at various scales.

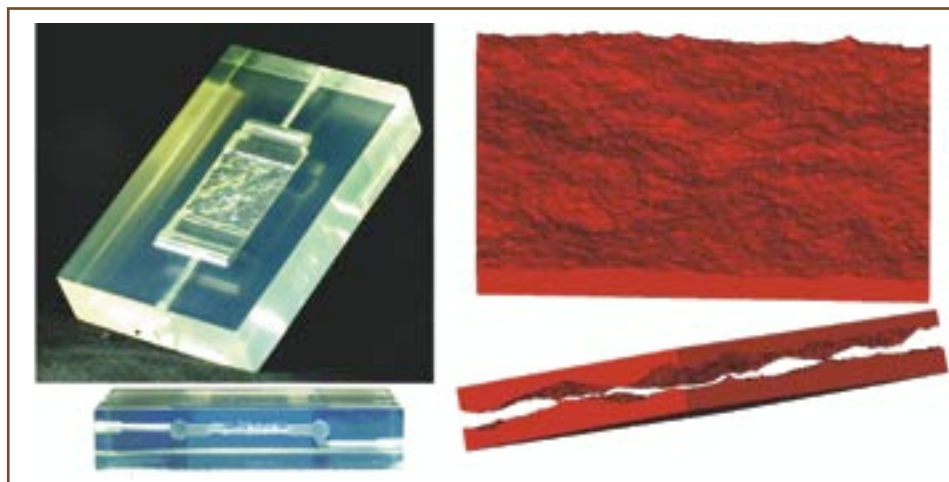
Stereolithography Opens Window for Fracture Flow Study

If all rocks were transparent, it would be simple to study their internal fractures and imperfections. Unfortunately, they are not, but stereolithography is the next best thing. Now, a team of INEEL researchers is utilizing stereolithography to study how biofilms form and affect flow in fractures.

"It seemed to me that stereolithography could be useful for subsurface research as a way of reducing experimental uncertainty," said INEEL optical physicist Vance Deason. "It offers tighter control of experimental conditions, which in turn gives researchers more certainty in interpreting the results."

Deason suggested the concept as a means to create highly controlled experiments on fluid flow in fractures.

"There is no question that biofilms can and do affect fracture flow, but until recently we haven't had the tools to study



Stereolithography allows INEEL researchers to study fracture flow with transparent three-dimensional physical flow cell models (front and side views of a model shown at top left). The models are based on computer representations (shown at in red at top right).

them," said INEEL microbiologist Daphne Stoner. "With stereolithography, we have the experimental window to study the interactions of microbes in fractures that we were missing. Now we just need to design the appropriate experiments to study the process."

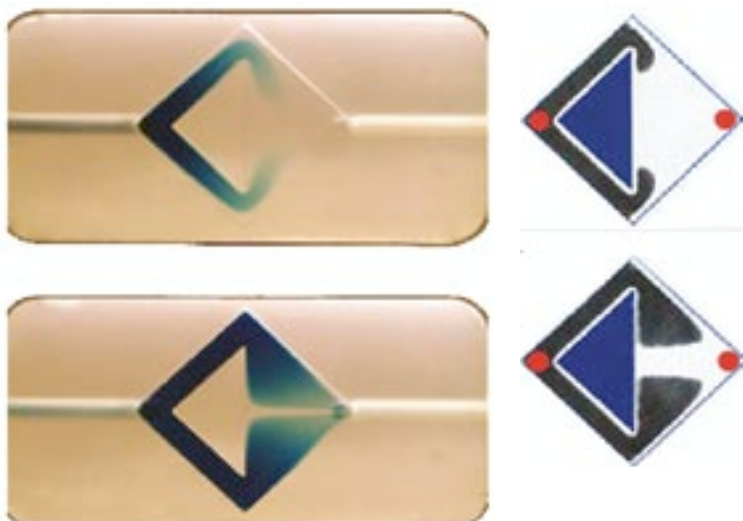
Generating stereolithographically fabricated flow cells for their research was the first step. For this, the INEEL team used various digital sources based on both

fractal models and actual rock fractures. (See *Stereolithographs—Models from Real and Virtual Fractures* on page 9.) They designed a variety of stereolithographs based on these fracture models. FineLine Prototyping, Inc., a company that specializes in stereolithography, fabricated them. Stoner and her team began preparing to study how biofilms form in fractures.

"Before we could begin to introduce biotic influences, we had to develop ways to collect information," said Stoner. "INEEL engineer Scott Watson built a data acquisition system that helps capture information about the dynamics of fluid flow in the surrogate fractures with and without biofilms."

The first experiment involved comparing real flow patterns in the flow cells (the stereolithograph prototypes) with those predicted by computational models. INEEL physicist Paul Meakin assisted the team by developing the fluid flow models for the specific stereolithographs the team studied. Through digital imaging, abiotic flow paths were established and compared with flow mechanics models calculated using Lattice Boltzman simulations. The initial results showed good correlation between

The flow of dye in a transparent three-dimensional stereolithograph (pair of images below left) is strikingly similar to flow patterns predicted by computational hydrodynamic models (below right).



actual flow patterns and those predicted by modeling.

Then the team began conducting experiments using a variety of flow cells to simulate the impact of microorganisms and biofilm on fluid flow within fractures. They pumped media suspensions of calcite precipitating microorganisms (*Shewanella putrefaciens* and *Escherichia coli*) into the flow cells at a range of flow rates and durations. A constant fluid flow through the cell was maintained with a computer-controlled syringe pump. Then, dye was injected into the lines to assess the fluid flow with and without biofilm.

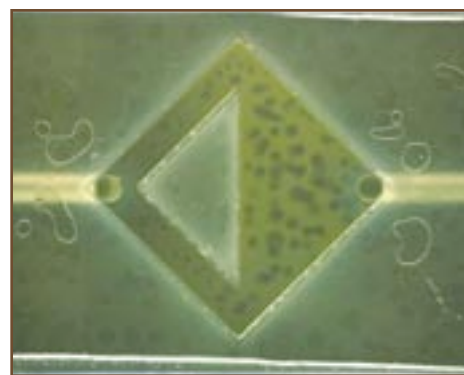
The biofilm growth was monitored and its impact on flow measured with

sensitive pressure transducers. Time-lapse sequences recorded the growth, providing visual correlation with modeled results.

The initial experimental results showed that biofilms do affect flow through the simulated fractures. The *E. coli* bacteria formed abundant biofilm growth, which could be seen without optical magnification, around the sides and corners of the cells. The growth diverted or slowed some fluid flow paths. The *S. putrefaciens* bacteria produced little biofilm formation and did not produce a significant change in the fluid flow.

“The microorganisms seem to preferentially attach to areas in the eddy

(Stereolithography continued on page 13)



The mottled texture in a digital image of a flow cell (above) represents *E. coli* biofilm, which formed behind a triangular obstruction when nutrients were injected into the water flow.

Stereolithographs—Models of Real and Virtual Fractures

A stereolithograph, essentially a transparent three-dimensional physical realization of a digital model, is produced using a laser and photocurable liquid resin. A single pass of the laser across a liquid resin surface effectively draws a solidified two-dimensional cross-section. Multiple passes result in a high-resolution (.05 millimeter) three-dimensional stereolithograph.

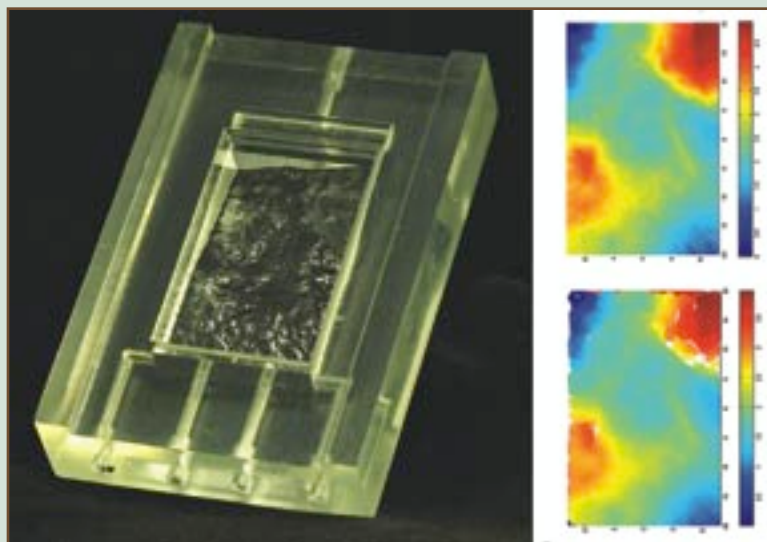
Using stereolithographs results in several benefits. Not only do researchers get precise physical models that offer a high degree of experimental control, but each model is based on a digital pattern, strengthening the connection between computational models and experimental work.

The digital models can either be produced from three-dimensional scans of real fracture surfaces or they can be generated by mathematical simulations. INEEL physicist Paul Meakin, recruited by the SSI to enhance its modeling efforts,

has generated simulated fracture surfaces by applying his knowledge of fractals. Meakin, author of *Fractals, Scaling and Growth far from Equilibrium*, is known for his work with the computer simulation of processes that lead to fractal structures.¹

“Fractal algorithms are often simple,” said Meakin. “But the resulting structures can be quite complex.” (See *Science Confronts Chaos and Complexity* on page 7).

Fractal geometries are “scale-invariant.” In other words, subsets of a self-affine object will look nearly identical to the whole as the spatial scale changes. Extensive experimental studies indicate that the fracture of brittle materials



A laser scan of a fractured rock surface (top right), which was used to generate the flow cell at left, closely matches an ultrasonic scan of the flow cell stereolithograph (bottom right).

generates self-affine fractal surfaces, and the property of self-affinity allows researchers to simulate fracture surfaces that maintain certain similarities at a variety of scales.

1. Meakin, *Fractals, Scaling and Growth far from Equilibrium* (Cambridge University Press, 1998).

Thinking Dynamically about Barriers

The future will be full of surprises—some are good, some not. When it comes to the performance of engineered barriers, surprises are best avoided. INEEL researchers are using systems dynamic modeling to develop a comprehensive computer model that will allow researchers to run simulations to improve the design and management of barrier systems.

“The design lifespan for engineered barriers ranges from 30 to 1,000 years,” said INEEL systems engineer Steve Piet. “There are a lot of changes over the course of a millennium, yet we design caps and barriers as though the environment is static. To improve their longevity, it is crucial that we better understand the full range of dynamics that affect them.”



Engineers are often required to make conservative and costly engineering choices to overcome uncertainties when designing barriers, such as the one recently installed at the INEEL CERCLA Disposal Facility (above). INEEL researchers are developing a systems dynamic model to reduce the cost and improve the performance of future barrier systems.

The government currently relies on engineered barriers at thousands of landfills and disposal facilities and will build more to contain hazardous materials. In many cases, engineered barriers will be a component of a final end state in which waste is separated from the environment for as long as it is hazardous.

Despite this critical role, engineered barriers have performance limitations and are subject to changing physical, biological

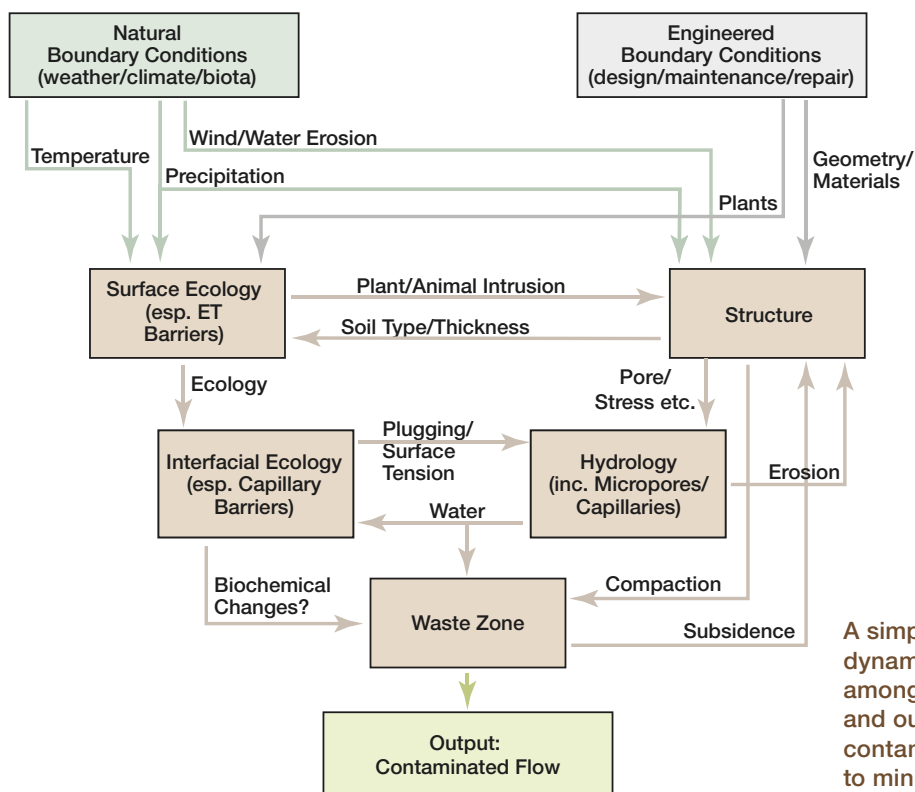
and chemical conditions. For example, prescribed designs that work well in humid climates can fail in arid ones.

“There is no question that it is a good idea to come up with cheaper barriers that maximize protection of the environment,” said SSI director Mike Wright. “They need to last longer, perform better and require less maintenance, but we need to improve our approach to the problem to do that.”

Piet, and a team of researchers from the INEEL, several universities and the private sector, are working on a systems dynamic model that factors in variables that other models typically treat as constants.

“Right now, a typical cap assessment treats the barrier’s structure as static prior to some defined lifetime,” said Piet. “It may consider time-dependent variables, such as temperature and precipitation, but it doesn’t consider how those and other variables affect the overall system.”

The model they are developing will also consider how various elements interact, such as plant ecology, capillary break interface, material properties and surface erosion rate.



A simplified diagram of the team’s conceptual dynamic model (left) illustrates the relationship among boundary conditions, state variables and outputs. The output is downward flow of contaminants, which the engineered barrier seeks to minimize.

"System dynamics is an analytical approach that examines systems by studying their underlying structure," said INEEL statistician and modeler Jake Jacobson, who has developed systems dynamic models for many other applications. "The approach allows us to make predictions about how the system will react to change."

Both Jacobson and Piet believe thinking about systems more dynamically is crucial to improving barrier designs and catalyzing a barrier improvement cycle (iterative learning and application) that improves performance management.

"As others have said, all models are wrong, but some are useful," said Piet. "Dynamic models provide new insights into the performance of these systems and complement existing hydrological and civil engineering models."

The team has already developed a numerical simulation that is designed to clarify the complex relationships among the various components within the cap system and the management practices that affect performance. Apart from offering a mechanism for continuous improvement, the systems dynamic model allows researchers to ping the simulation with perturbations to see how it responds.

Other engineering fields have learned the hard way that excessive complexity and failure to understand dynamic interactions can lead to poor and sometimes costly predictions.

"It is important to consider feedback," said Piet. "Whether you are designing an airplane, a nuclear reactor or an engineered barrier, we know that system failures occur when we fail to consider interactions. The advantage of dynamic modeling is that we can simulate feedback and shore up those aspects of barrier design that strengthen performance while mitigating factors that weaken it. The output of our work will be barrier designs that keep getting better."

The INEEL is currently conducting a number of projects that examine nearly every aspect of barriers. They include studying how they hold up through time (see *Freezing the Assumptions Out of Geosynthetic Clay Liners* on page 14), improving the understanding of factors that can strengthen their design (see *Design Issues that Afflict Barriers* on page 12) and developing better systems to monitor them (*Geophysical Monitoring System Installed at EPA's Gilt Edge Superfund Site*, **SubsurfaceTopics**, March 2003).

"Nature will win eventually," said INEEL ecological engineer Bob

Breckenridge. "By better understanding the interaction of nature and barrier systems, we can work with nature to provide better protection for long time periods at less cost."

Contact: Steve Piet, Sc.D.
208-526-5252
pietsj@inel.gov

Robert P. Breckenridge
208-526-0757
rpz@inel.gov

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■ (Sol Lynn continued from page 15)

is not capable of factoring in the vertical interaction of contamination in each zone and assumes uniform hydrological properties for the entire site.

Arnett's final task was developing an understanding of the results. "Once the parameters are determined, the next challenge for scientists is not running the code, but interpreting what the model tells you," said Arnett. "That is where experience helps."

"Modeling can be more art than science. Without a good understanding of the assumptions that go in and the

limitations of the particular model, managers can overly trust or entirely dismiss the results. My job is finding the realistic balance point between those two extremes."

Now, with the work completed, Arnett and his colleagues have a better understanding of the nature and extent of the Sol Lynn plume and the implications for remediation. Unfortunately, in their assessment, the native microbes beneath the Sol Lynn site don't appear to be sufficiently effective at degrading TCE on their own.

"The plume is still expanding in some water-bearing zones," said Arnett. "Based on our modeling work, I suspect it will take more than monitored natural attenuation to contain it at the source."

Contact: Ken Moor
208-526-8810
ksm@inel.gov

This research is funded by the U.S. EPA, Region 6. It is being conducted by Ron C. Arnett (of the INEEL) in collaboration with Roger W. Lee (of the USGS).

Addressing Design Issues That Afflict Barriers

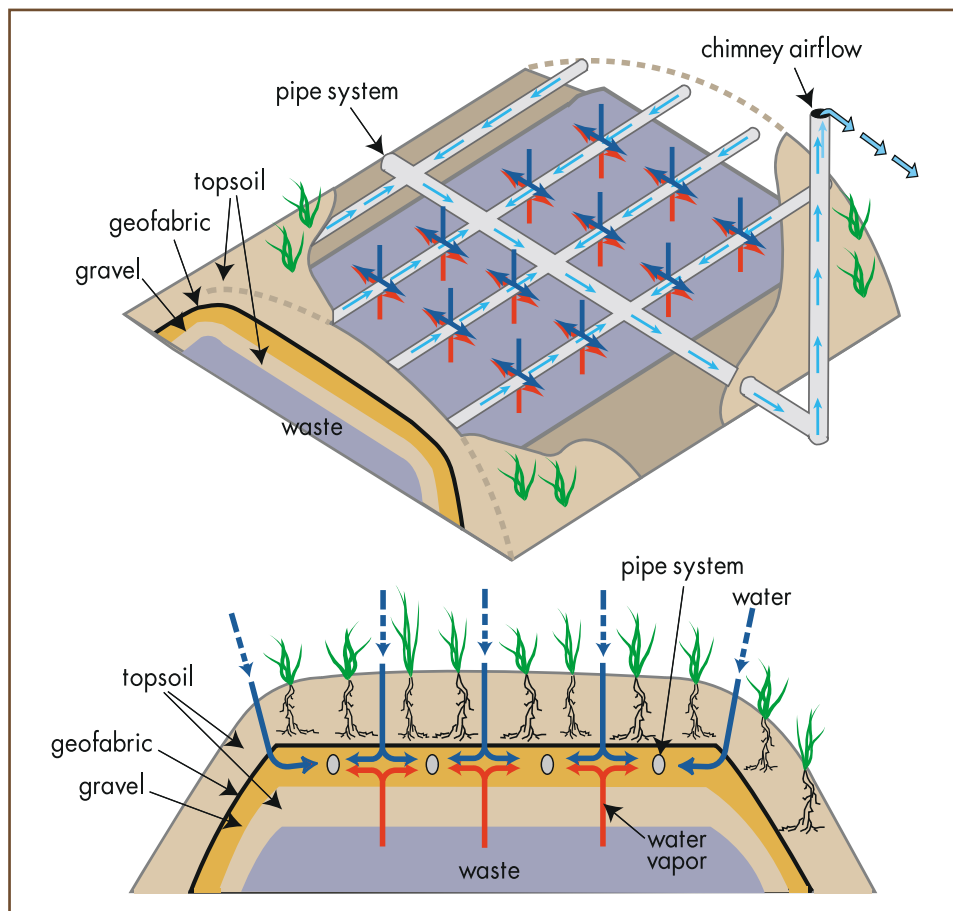
Engineered barriers are supposed to prevent contamination from reaching the environment, but sometimes they have the opposite effect. INEEL scientists are working with regulators, other researchers and the private sector to identify and fix the specific conditions and design issues that can turn barriers into environmental problems.

Mark Ankeny, the new INEEL geosciences group manager, believes the regulatory requirements for barriers are so focused on keeping water out of systems that they fail to take into account what happens within them.

"I think the root of the problem is simple," said Ankeny. "We don't always know what we are doing and don't consider all of the reasons why we are doing it."

Ankeny, who has years of experience as a researcher and consultant in the design and construction of landfill caps, believes the problem is rooted in the original RCRA focus on designs for the wetter environments of the eastern United States. Designs were based on avoiding "bathtubbing"—a situation that results when water is unable to leave an area as fast or faster than it enters it. Given the vision of floating waste, rotting, forming leachate or spilling into groundwater or surface water, it made sense to design a barrier whose cover had lower permeability than its liner.

Unfortunately, the physics of the design often produces an unintended consequence—"gastubbing." Covers designed to prevent water from entering the system also tend to restrict oxygen. So paper, yard waste and other organic matter in many landfills are anaerobically



Soil carburetor designs are one way to overcome the problem of "gastubbing" in barriers. Gases in the system are distributed with an inexpensive embedded perforated pipe system, giving managers greater control of the chemical conditions beneath the cap.

decomposed. When the methane and carbon dioxide produced by microbial breakdown cannot adequately exit through the liner, even when the cover is vented, some gases are forced downward, carrying organic solvents and sorbed metals into the vadose zone or groundwater.

"When volatile organic compounds and methane are forced into the vadose zone, the conditions result in the reduction of metals and the oxidation of methane," said Ankeny.

Methane and carbon dioxide production also results in a complex set of secondary effects. In caps with vegetative covers, the upward-moving gas displaces the oxygen that plants need to maintain healthy roots. The oxygen stress effectively shuts down plant transpiration

and allows more water to infiltrate downward into the underlying waste, resulting in even more gas production.

A greater problem is the extremely reducing system beneath the cap, in which oxygen is stripped from insoluble metal oxides, making them more mobile. Again, the secondary effects are complex.

"Iron is common in soils, but when it is reduced, it frequently carries some sorbed arsenic with it," said Ankeny. "One product of oxidizing methane and reducing iron in soil is the production of water beneath the cap."

Ankeny estimates that some systems are capable of producing water in quantities equivalent to several centimeters of precipitation. Though it may seem insignificant, it is essentially

rainfall inside the cap and can't be vented from the system by evapotranspiration.

"By neglecting the gas portion of the equation, waste products are trapped and have nowhere to go but sideways or down," said Ankeny. "That means a cap can actually serve to drive contaminants toward the water table. Of course, this wasn't what regulators or the designers had intended, but it is commonly what they get."

Ankeny's colleagues, ecological engineer Bob Breckenridge and systems engineer Steve Piet, cite this as an example of the "law of unintended consequences," when by solving one problem apart from its larger context, other problems are created.

To overcome these issues, Ankeny believes the science of landfill design needs to incorporate or simulate systems that actually have waste beneath them. One reason unintended consequences have occurred was because the early research on landfill cover designs was typically conducted without waste beneath the test plots. It wasn't considered necessary

because the goal was to see how well a cap could keep water out of the waste.

The INEEL team's goal is to design barriers that are simpler, less expensive, longer lasting and easier to monitor by considering the dynamic interactions between natural systems and engineered components.

"We need to go back to the root of the problem, redefine the requirements for caps and base them on the science of what occurs from a system perspective," said Ankeny. "That presupposes we have already done the science, but we are still working on that."

According to Ankeny, mesoscale facilities are ideal for conducting realistic experiments that include waste as part of the system. "If we simulated the geometry and stoichiometry of a landfill system in a laboratory setting, we could obtain the information we really needed when we originally defined cap performance parameters," said Ankeny.


In the meantime, Ankeny has designed and installed some practical intermediate

solutions. One solution for venting gases works similarly to a gas carburetor. It has the potential to allow managers to manipulate the chemical conditions inside the landfill system.

Overall, Ankeny thinks it is more important to fix the problem, not the blame. "When the regulations were written, best management practices were based upon the best research at the time, which was mostly performed in wetter climates," he said. "Now that we see that our first concepts have some negative consequences, it's our duty to correct the problem. That opportunity is a big part of what brought me to the INEEL."

*Contact: Mark Ankeny
208-526-5748
ankemd@inel.gov*

Note: This research is funded by the Environmental Systems Research and Analysis (ESRA) program and conducted by Mark Ankeny, Ph.D.

 (Stereolithography continued from page 9)

regions behind micro-obstacles in the flow path," said team member and INEEL biologist Robert Stedtfeld. "But we need more sensitive pressure transducers to more precisely quantify the results."

As results stream in, the team will continue comparing experimental runs with a variety of computational models.

"The first set of experiments used a stereolithograph with a very simple shape," said Stoner. "The next set will use much more complex prototypes with multiple flow pathways that can become clogged and reroute flow. Biofilms introduce complexity to the system behavior that we hope to be able to model." (See *Fracture Flow Dynamics—The Building Blocks of Understanding Fractures* on page 3.)

Stoner's plans for this research are to eventually use synthetic rocks that more closely represent the chemistry of basalt. The synthetic rocks could be created using an approach similar to standard stereolithography, in which a laser is used to polymerize a liquid monomer, by fusing an inorganic powder, such as pulverized basalt.

"Because microbes can preferentially attach to certain minerals, our simulations will need to mimic the natural environment as closely as possible," said Stoner. "If we lose optical transparency by adding minerals and metals to the stereolithographs, we can use other imaging techniques to monitor biofilm growth and fluid flow in the system."

Besides providing huge insights, stereolithography and its usefulness in studying biofilms and fracture flow is a research gold mine. "We are just getting started and already have a lot of papers in the works," said Stoner. "As results come in, it will only get better."

*Contact: Daphne L. Stoner
208-526-8786
dstoner@inel.gov*

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Freezing the Assumptions Out of Geosynthetic Clay Liners

An engineered barrier's life span is based on knowing the life span of each of its components. Without that knowledge, engineers are either forced to make assumptions, which increases uncertainty, or add conservatism, which increases costs. However, new knowledge about one common component's ability to withstand repeated freezing and thawing will soon be available when INEEL geoscientist Robert Podgorney and his collaborators complete a study of geosynthetic clay liners (GCLs).

Developed in 1986, GCLs are a relatively new technology for meeting federal standards for landfill barrier systems. They consist of a thin layer of processed clay (typically bentonite) that is either bonded to a geomembrane or fixed between two sheets of geotextile.

They have numerous advantages over traditional compacted clay liners, which have made them increasingly popular with

engineers and regulators. Not only are they cost-effective when clay is not readily available, they are fast and easy to install, have low hydraulic conductivity and are "self-healing." After installation, the clay swells as it hydrates, and seals rips and holes up to 75 millimeters in diameter while retaining its effectiveness.

However, there are still several unknowns, including whether GCLs' low permeability is effective for their assumed design life. For example, current data only suggest that their hydraulic conductivity is unaltered after five freeze/thaw cycles.

Three well-known types of GCLs were chosen for the study: Claymax® 600CL, Bentomat® ST, and Bentomat® DN, all developed by CETCO Lining Technologies Group.

Claymax® 600CL is a nonreinforced GCL commonly used for flat areas of landfill caps and high hydraulic head conditions in bottom liner applications. It consists of two lightweight geotextiles that encapsulate a sodium bentonite layer with a composite laminate applied to one of the geotextiles. Bentomat® ST is similarly

designed, but reinforced, which permits its use in a wide variety of field conditions. Bentomat® DN is similar to Bentomat® ST, but has a high-friction interface that makes it better for steep slope liner/cover systems.

Podgorney's team has already completed more than 80 freeze/thaw cycles, more than four times the number reported in the research literature.

"For our experiments, we are assuming three freeze/thaw cycles are equal to one calendar year of field exposure," said Podgorney. "We have instrumented a field site to check this assumption and should have data this winter, but it is safe to say that the existing data on performance haven't caught up with the age of the technology."

Podgorney and his colleagues expect to complete a total of 150 freeze/thaw cycles by the end of 2003. If their funding continues, they hope to eventually complete as many as 300 cycles, which is reasonably equivalent to a 100-year period in some INEEL locations.

Podgorney recently started post-exposure testing and is optimistic about the eventual results. "Though we aren't finished, my preliminary assessment is that the GCLs seem to be holding up well. Our final conclusions, which we intend to publish in a peer-reviewed journal after they have been validated, will provide engineers and regulators much greater certainty on one of the more critical components of modern barrier systems."



INEEL geoscientist Robert Podgorney uses a set of permeameters to study how well geosynthetic clay liners perform after numerous freeze/thaw cycles. So far, more than 80 freeze/thaw cycles have been completed, more than four times the number reported in the research literature. Though the study is not yet complete, Podgorney's preliminary assessment of the GCLs' performance is positive.



Contact: Robert Podgorney
(208) 526-1224
podgrk@inel.gov

This research is funded by Environmental Systems Research and Analysis (ESRA) program and conducted by R. Podgorney, in collaboration with G. Stormberg, J. Bennett and S. Piet, Sc.D.

Modeling the Sol Lynn Plume

Despite a five-year pump-and-treat effort, a trichloroethylene (TCE) plume in the groundwater is still expanding northward under a Texas freeway near the Houston AstroDome. At least, that's the assessment of INEEL chemical engineer Ron Arnett. He and hydrogeologist Roger Lee of the U.S. Geological Survey (USGS) have modeled the plume's extent and movement. They have determined that the TCE source area will not degrade readily on its own without further remediation.

The plume originates at the one-acre Sol Lynn/Industrial Transformers Superfund Site, situated in an urban part of Houston. From the mid-1960s until the mid-1970s, two businesses were located at the site—first a company that reclaimed wire and electrical transformers and then a chemical supply company—and both PCBs and solvents were dumped onsite.

Because of the soil and groundwater contamination, the U.S. Environmental Protection Agency (EPA) added the site to its National Priority List of Superfund sites in the early 1980s. It is estimated that more than four million gallons of groundwater are contaminated. TCE, the principal groundwater pollutant, is found in concentrations of up to 790 parts per million in shallow aquifer wells less than 80 feet deep.

In 1993, the EPA began a pump-and-treat operation to remediate the groundwater. After five years of operation, it was apparent that the TCE levels in the groundwater were not being reduced as projected. The EPA halted the extraction process and began looking for a new solution.



INEEL chemical engineer Ron Arnett's recent assessment of a trichloroethylene (TCE) plume originating at the Sol Lynn/Industrial Transformers Superfund Site is that the plume is still expanding despite a five-year pump-and-treat effort. The Sol Lynn site is located in a well-developed area of Houston, Texas. Approximately 2,100 people live within a one-mile radius; four private and four city water wells, serving more than 10,000 people, are within a three-mile radius; and the Houston AstroDome and recreational facilities are less than a half-mile away.

In 2001, the EPA and the Texas Natural Resource Conservation Commission began a second investigation. It was during this period that the EPA asked Arnett to help further characterize the site and identify the remaining source of TCE and the solute plume.

"INEEL's experience with TCE biodegradation and groundwater modeling was something EPA was looking for," said Ken Moor, who manages INEEL's Superfund Technical Support program.

"The fact that levels didn't drop as expected indicated there was a problem with residual DNAPL," said Arnett.

According to Arnett, the hydrogeological system beneath the Sol Lynn site is not simple. The top 100 feet of the subsurface consists of eight to nine water-bearing zones of silt and clayey silt. The TCE is principally confined to the upper four zones, with the apparent residual DNAPL source located in the north-central part of the site. There is communication among the top four zones, but each zone is a separate system with its own flow properties.

After additional monitoring wells were installed, Arnett and Lee began collecting data with the help of other EPA contractors so a conceptual model for the site hydrogeology could be developed.

Data was collected on contaminant concentrations, aquifer properties and biodegradation rates for each zone. Source areas were identified by their high concentration of TCE. Biodegradation potentials were determined by measuring the presence of reductive dechlorination byproducts, produced naturally when native microbes degrade TCE to other compounds.

"With a freeway cutting across the plume, we weren't always able to get the monitoring wells where we wanted them," said Arnett. "However, we got the data we needed."

Arnett then developed BICHLOR models, which are capable of simulating the reactive transport of TCE and accounting for biodegradation in multiple reaction zones. However, because the BICHLOR model is one-dimensional, it

(Sol Lynn continued on page 11)

INEEL Hosts Distinguished Geoscientists

Geocentrifuge Workshop

The INEEL hosted a workshop in Idaho Falls in late March to introduce its new Geocentrifuge Research Laboratory to the scientific and engineering community. The new facility features a 2-meter radius, 50 g—tonnes (metric ton) capacity geocentrifuge and is one of the few worldwide primarily dedicated to geo-environmental applications.

“INEEL’s geocentrifuge is a major asset for researchers in the region, but only if they know it is here and how to use it,” said Alan Stadler, lead researcher at the facility. “One reason we hosted this workshop was to share information about the research we’re planning and are interested in conducting. We also wanted to let participants know how instruments similar to ours are being used around the country and describe our instrument’s particular capabilities.”

The workshop participants discussed specific research projects as well as the strengths, weaknesses, possibilities and challenges of performing experiments with

the new geocentrifuge. Featured were guest speakers from the Massachusetts Institute of Technology; University of California, Davis; University of Colorado, Boulder; Bechtel National, Bechtel Savannah River; University of Idaho and the U.S. Army Corps of Engineers.

Animating Plate Tectonics and Other Geologic Stories

In late May, the INEEL hosted National Academy of Sciences member Tanya Atwater, who is renowned for her pioneering research in tectonic evolution of western North America and the San Andreas fault system. Atwater, from University of California, Santa Barbara, presented a seminar titled *Animated Plate Tectonics of the Western United States*.

According to Atwater, she now has a higher calling—teaching. “To many of my colleagues, my current passion and focus on teaching, education and outreach looks like a regression,” said Atwater. “But what good is research if the audience that finds it interesting is getting smaller and smaller. I want to share my love for geology with people in a way that makes all of our research more meaningful.”

Atwater shares her passion for geology using creative multimedia presentations that mix photos of recognizable landmarks

and landforms with animations that dynamically explain their geological origins. This work has earned her the prestigious Director’s Award for Distinguished Teaching Scholarship, the highest honor given by the National Science Foundation for excellence in both teaching and research.

With her students’ and colleagues’ support, Atwater is now establishing the Educational Multimedia Visualization Center (EMVC) at the University of California, Santa Barbara. She envisions that scientists will be able to bring their ideas to the EMVC and gain the technical expertise they need to produce similarly dynamic and creative computer animations for teaching and outreach.

“Anyone with the need to tell a geological story rooted in solid scientific research is invited to use the center,” said Atwater. “We want you to be able to bring your work to life with animation.”

Contact: Tanya Atwater, Ph.D.
atwater@geol.ucsb.edu

Note: More information about the EMVC is at <http://EMVC.geol.ucsb.edu/>

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